Materials 286G: Assignment 4

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You can work in teams of up to 2 people and submit a single assignment from each team.

You need: R_0 for Mg^{2+} and O^{2-} = 1.693; R_0 for Zn^{2+} and O^{2-} = 1.704; B = 0.37.

1. Use this information to calculate equilibrium distances between Mg and O in the zinc blende, rock salt, and CsCl structures. Make a plot of distance between Mg and O as a function of V_{Mg}/Z, *ie.* bond length *versus* bond strength, where V_{Mg}, the Mg valence is 2, and Z is the coordination number (4, 6, or 8). For rock salt, compare with experiment.

2. DFT problem: Determine the relaxed cell parameters for these structures. Compare with all of above.

3. In the above three structures of MgO, vary the equilibrium distance in steps of 0.5% from -3% to 3% and make a plot of the instability index with distance. The instability index G is given by:

$$G = |V_{Mg} - S_{Mg}|$$

   where S_{Mg} is the calculated bond valence sum of Mg.

4. DFT problem: Calculate the total energy of either rock-salt MgO or zinc blende MgO as a function of the same step-sizes and overlay the plot of energy *versus* distance on the corresponding instability index plot.

5. The wurtzite structure of ZnO (space group $P6_3/mmc$) has Zn $(\frac{1}{3}, \frac{2}{3}, 0)$ and O $(\frac{1}{3}, \frac{2}{3}, u)$ with u near $\frac{3}{8}$. Note that there are two kinds of Zn–O distances; three to the O at the base of the O_4 tetrahedron, and one to the O at the apex. Optimize the ZnO structure by minimizing the instability index as defined above. You may need to start by fixing u to the ideal value and then changing a and c near the values of a = ≈3.2 Å and c = ≈5.2 Å. Make appropriate 2D plots ! Once a and c are determined, vary u and make a plot of G *versus* u.